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RESEARCH ARTICLE

Importance of geometric parameters in modeling of porous materials – a finite element study

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Abstract

Porous materials consist of interconnected skeletal structure around a porous space. The skeletal structure is usually formed of a solid phase and the pores are typically filled with a fluid (liquid or gas). Porous materials are characterized by two essential geometric properties: porosity and pore size distribution (PSD), which influence their bulk mechanical properties. Porosity, which is defined in terms of the ratio between the envelope and the skeletal densities, is sufficient to describe the elastic bulk properties of porous materials. Gibson and Ashby developed a power scaling law expressing the linear relation between the elastic modulus and the relative density. The PSD describes the spatial variation of the pore sizes and has recently been shown to influence the mechanical properties of porous materials. In addition to porosity and PSD, the pore characteristics, namely pore size and shape, and pore-wall size and shape, also determine the geometric properties that influence the bulk response of these materials. In this study, the importance of the above-mentioned geometric parameters in the modeling of the porous materials is studied using a computational framework. The bulk mechanical response under large deformation of various porous structures with PSD based on different probability density functions (PDF) and different combinations of other geometric properties under uniaxial compression is investigated. The sensitivity of mechanical response to these geometric parameters is studied. Interdependent parameters which are significantly influential are identified. By controlling these parameters, the synthesis of porous materials can be guided and optimized.

1 | INTRODUCTION

Due to the increasing cost of raw materials and advancement in sustainability, reduced materials consumption in different applications is a major challenge. Thus, the state-of-the-art in engineering applications is the use of lighter and innovative construction materials with excellent properties. One such promising material types are nanoporous materials. Nanoporous materials have the most favorable applications and proved to be satisfactory for their applicability due to their high stiffness-to-weight ratio, better crash energy absorption, low thermal conductivity, and lower density. Along with drastic weight reduction and material savings, there are other application-specific benefits like acoustic & mechanical damping, energy storage, and filtration effects [1]. In nanoporous materials, pores are enclosed within a solid phase made up of either organic or inorganic materials and are generally classified as open or closed pores. Open porous material consists of an interconnected skeletal network around the void space in such a way that the pores connect to the surface of the materials, while closed porous materials consist of pores enclosed within the bulk phase.

Generally, nanoporous materials are brittle under tension and undergo large-strain plastic deformation exhibiting significant energy absorption behavior under compression. This requires research into their mechanical properties under compressive loading conditions. The bulk mechanical properties of nanoporous materials depend on their microstructural properties, namely porosity, that is, the ratio between the envelope and the skeletal densities, and pore size distribution (PSD), which describes the spatial variation of the pore sizes within the microstructure [2]. Other pore characteristics, namely, pore shape and pore-wall size, also determine the geometric properties that influence the bulk response of these materials [3, 4]. The structural properties of nanoporous materials can be tailored during the manufacturing process according to the application requirements. For a better perception of the structure-property relationships, several experimental investigations are carried out extensively over the years, in a view to understand the influence of various synthesis parameters and optimize such materials with expected mechanical or thermal properties. However, computational modeling is a cost- and resource-efficient way in comparison with experimental testing. The most widely used methods for the reconstruction of porous materials are tessellations methods, namely Voronoi tessellations and Laguerre-Voronoi tessellations. Recently, Chandrasekaran et al. [5] proposed Laguerre-Voronoi tessellation (LVT) based on random closed packing of polydisperse spheres (RCPPS) to reconstruct the 3-d nanoporous microstructure of biopolymer aerogels. This model accounts for complex pore-structure inheriting the realistic PSD and shows qualitative agreement with experimentally obtained bulk mechanical response under compression. In this work, open-porous cellular-like structures with different structural properties are developed using the computational framework proposed in ref. [5] and their influence on the bulk mechanical properties under compression is studied using finite element methods (FEM).

2 | METHODS

A periodic Voronoi diagram representing a 3-d open-porous structure inheriting the given PSD is generated using RCPPS and LVT as described in ref. [5]. In addition, a structure with given porosity is obtained by defining appropriate cross-sectional properties to the cell walls of the Voronoi structure. The method of determining the cell wall diameter (CWD) for given porosity is illustrated in ref. [5]. The resulting Voronoi structure is transformed into a cube-shaped representative volume element (RVE) with periodic boundary conditions (PBCs) as illustrated in ref. [6]. An RVE in combination with PBCs has the potential to obtain the homogenized macroscopic response. Subsequently, the RVE was subjected to monotonic compression loading and simulated using LS-DYNA implicit finite element solver according to the FEM framework described in ref. [5]. Throughout this study, an elastic material model with Young's modulus (E) of 4.5GPa [7] is defined to characterize the behavior of the cell wall with a skeletal density of 1.72 g/cm^3. Porous materials are experimentally characterized based on the PSD, that is, the volume share of each pore size in the given system. Similarly, based on the PDF (which describes the number of occurrence of the pores in the system), the PSD is derived according to ref. [8]. To this end, an RVE with 1000 number of cells corresponding to symmetric beta distribution ($\alpha = 5, \beta = 5$) with mean pore width of 53 nm and standard deviation (SD) of 13 is shown in Figure 1. The RVE has a porosity fraction of 0.95. The comparison of the desired PSD (input to sphere packing algorithm) and the PSD of the resulting structure (as shown in Figure 1) is shown in Figure 2.

In this work, the investigated volume is limited to a RVE, which is small enough for achieving bulk response on a computer, but large enough to deliver a reliable result. Therefore, an RVE size that is large enough and computationally efficient has to be identified for a given PSD and porosity, so that any volume of an increased size will be equally representative having identical PSD. To this end, the representativeness of an RVE is studied based on the structural properties and the effective mechanical properties characterized by the model. The statistical properties of the PSD of the structure, that is, mean and pore width range, are compared for different RVE sizes and the respective structural properties, that is, CWD and effective macroscopic properties, are evaluated.

Based on this study, the most favorable RVE size is chosen, which is computationally efficient and shows convergence on the effective macroscopic properties of the structure. Therefore, RVEs with varying sizes, namely 250, 500, 1000, 2000 and 3000 cells, are generated based on symmetric beta PDF ($\alpha = 5, \beta = 5$) with a porosity fraction of 0.95. From Figure 3 and 4,

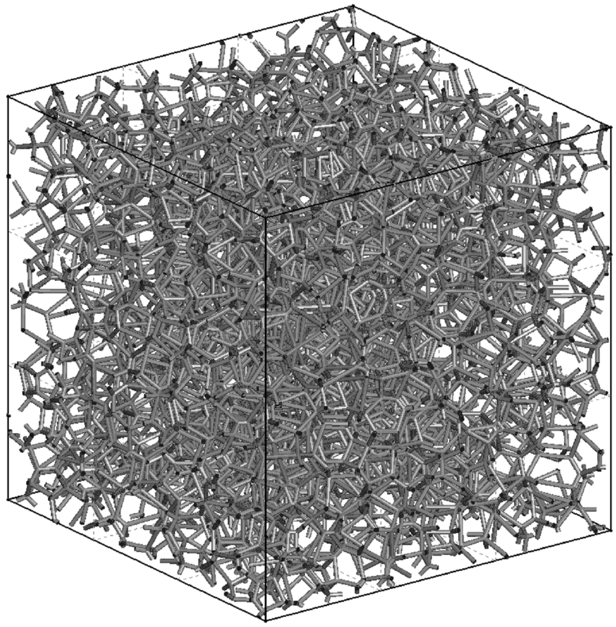

FIGURE 1 An example of an RVE with 1000 number of cells (N) having PSD shown in Figure 2. PSD, pore size distribution; RVE, representative volume element.

we infer that the statistical properties of the PSD for increasing RVE size converge, resulting in identical average CWD and effective bulk response. The choice of RVE size depends on the type of distribution and the pore width range considered, for example, a left skewed distribution requires a larger RVE size compared to a right skewed distribution due to more number of larger cells in the former than in the later. Therefore, if the RVE of any size inherits the complete description of the given PSD distribution, then it can be taken as a representative model of the real structure. In this work, the minimum RVE size for different PSDs is decided based on this convergence study. In order to study the influence of the three structural parameters, namely PSD, porosity and CWD, on the bulk mechanical response, two use cases were investigated as listed below:

Case I: Effect of porosity and CWD for a given PSD
Case II: Effect of PSD for a given porosity based on
- PSD corresponding to PDFs with varying mean
- PSD corresponding to PDFs with varying SD

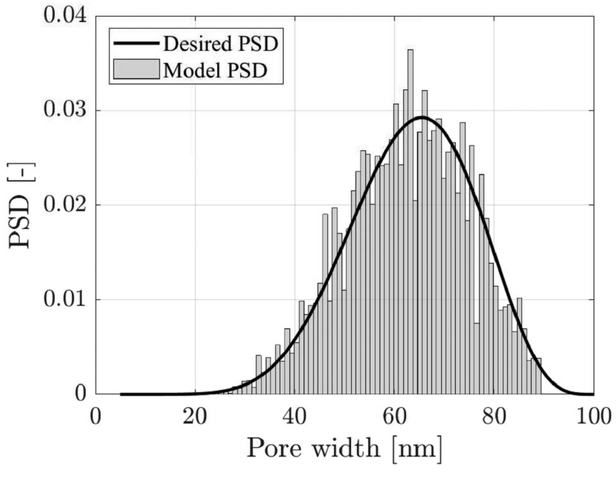

FIGURE 2 Comparison of PSD of the RVE model (shown in Figure 1) in comparison to the desired (input) PSD corresponding to symmetric beta PDF ($\alpha = 5$, $\beta = 5$). PSD, pore size distribution; RVE, representative volume element.

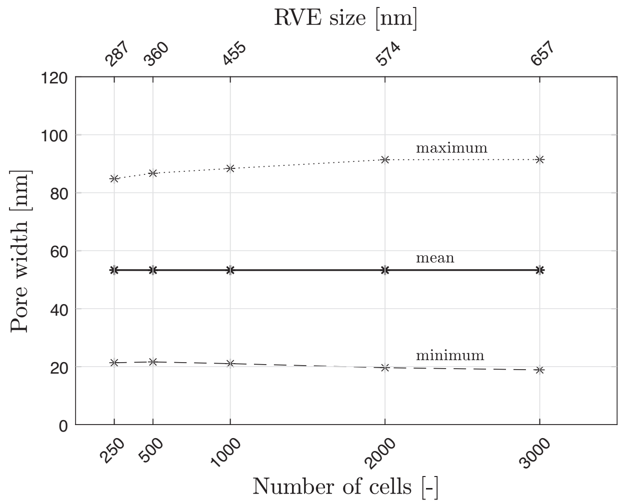

FIGURE 3 Convergence study on the statistical properties of the PSD for different RVE size/number of cells(N). PSD, pore size distribution; RVE, representative volume element.

3 | RESULT

In this section, the effective bulk response of the microstructure model (RVE) under compression for different geometric properties, namely PDF, CWD and porosity, are discussed.

3.1 | Effect of porosity and CWD

By increasing the average CWD, the porosity of the structure decreases as shown in Figure 5A, which eventually increases the solid fraction (i.e., the fraction of total volume taken up by the solid phase by which the structure is made). From Figure 5, we notice the following influence on the bulk mechanical response as the solid fraction increases, namely,

- Bulk stiffness of the structure increases
- Span of plateau regime decreases
- Strain at which the densification begins decreases due to earlier pore collapse

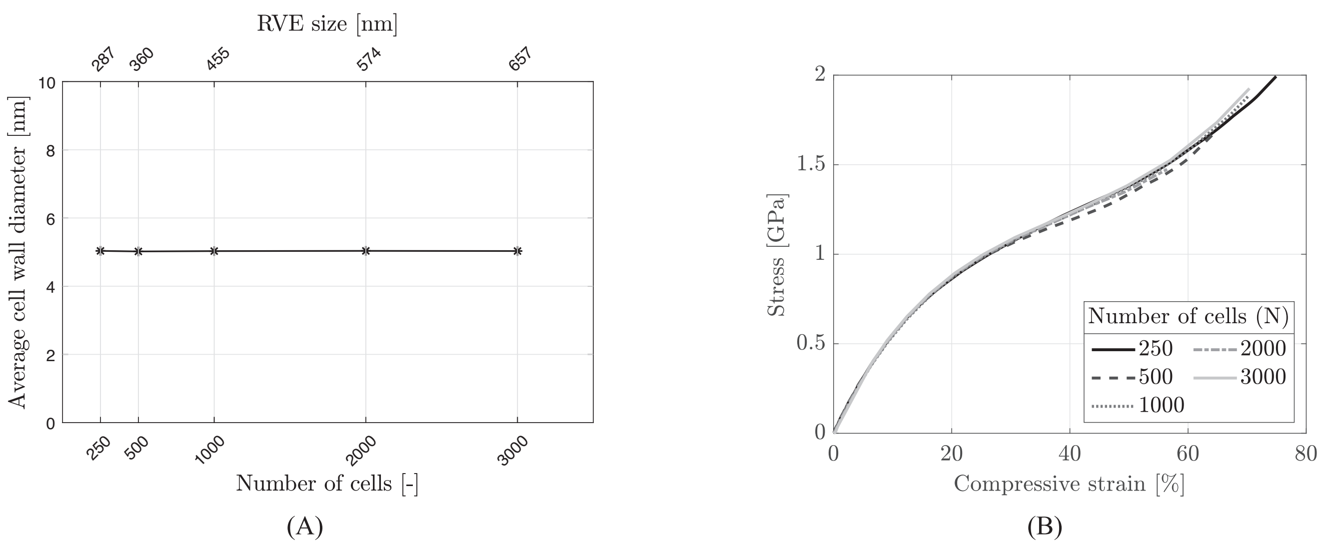

FIGURE 4 Convergence study on (A) average CWD and (B) effective mechanical properties of RVE with different sizes/number of cells(N) and constant PSD corresponds to symmetric beta PDF ($\alpha = 5, \beta = 5$). CWD, cell wall diameter; PSD, pore size distribution; RVE, representative volume element.

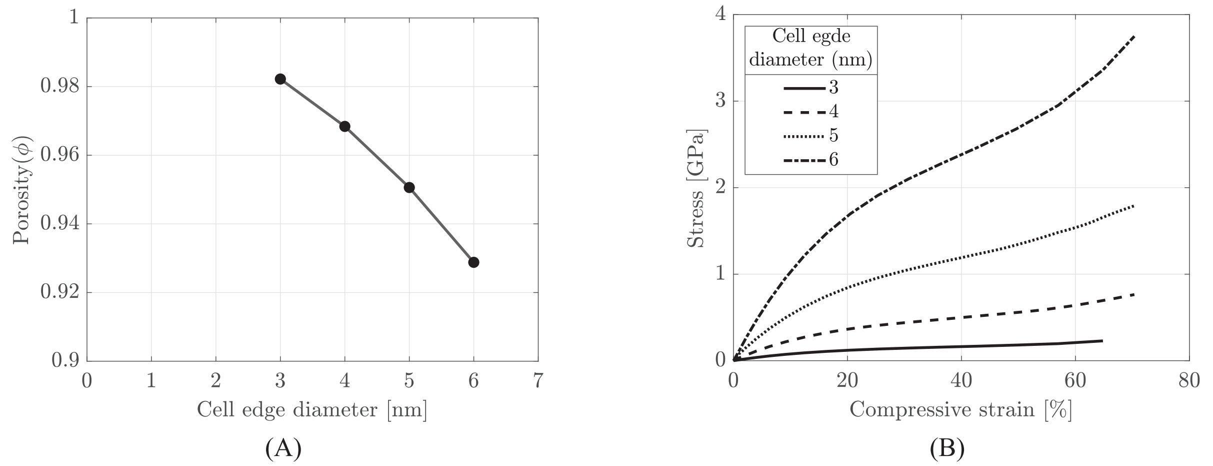

FIGURE 5 (A) Correlation between CWD and porosity (B) Comparison on the bulk response of the structures with decreasing porosity. CWD, cell wall diameter.

3.2 | Effect of PSD

In this section, the effect of PSD on the bulk mechanical response is studied based on different PDFs with varying mean and SD.

3.2.1 | Varying mean and constant SD

The different PSDs having constant standard deviation (SD = 7) and different mean pore widths (namely 40, 50 and 60) using normal PDF are compared in Figure 6A. As the mean is increasing the pore width range increases for a constant SD. As mentioned in methods section, the RVE size is different for each mean and is decided based on the convergence study.

From Figure 6B, we see that there is no influence of PSD on the bulk response of the structure under compression. This is because all the structures have identical PSD in the normalized scale as shown in Figure 7. As we increase the mean keeping the SD constant, the pore width range (minimum & maximum) is shifted accordingly and thereby also increases the RVE size. As a result, CWDs scale to the equivalent percentage of increase of the mean pore width in order to have the same porosity of the structure. Therefore, for a given solid fraction and PSD, the bulk response is unchanged in different scales.

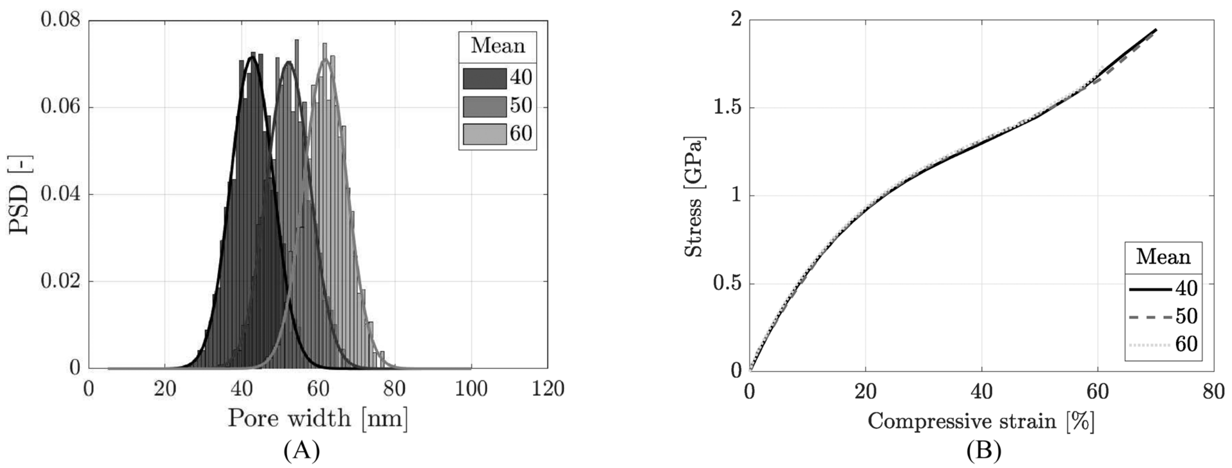

FIGURE 6 Comparison of (A) PSDs based on normal PDFs and (B) Bulk response of the structure with PSDs corresponding to Figure 6A, for different mean pore widths and constant SD. PDF, probability density functions; PSD, pore size distribution; SD, standard deviation.

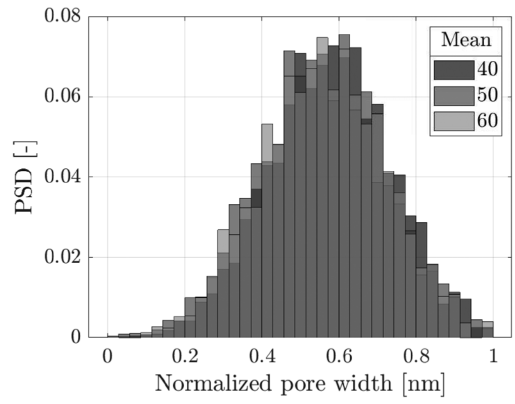

FIGURE 7 PSDs corresponding to Figure 6A with pore widths in normalized scale. PSD, pore size distribution.

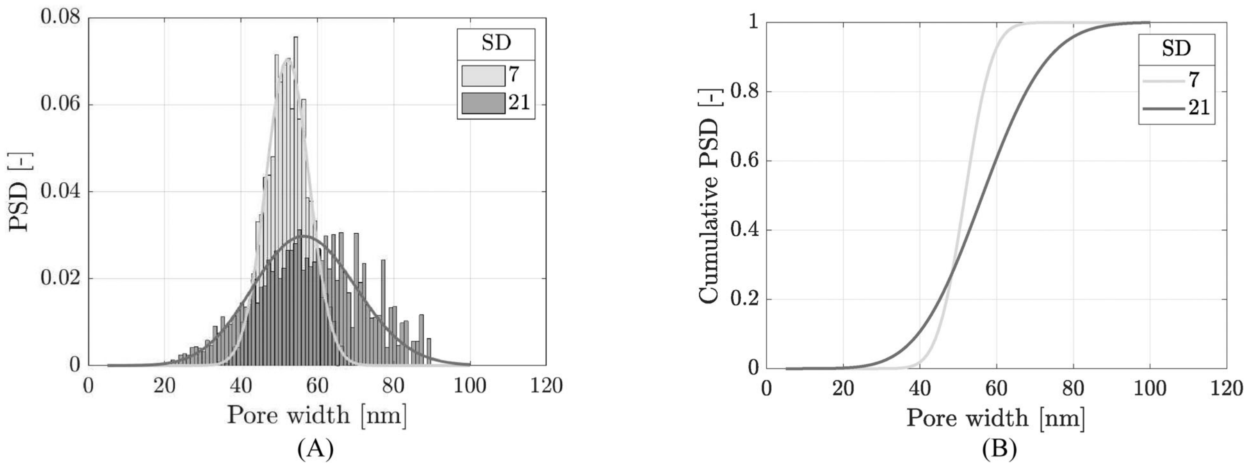

FIGURE 8 Comparison of (A) PSDs and (B) Cumulative PSDs with different SD and same CWD for given constant porosity. CWD, cell wall diameter; PSD, pore size distribution; SD, standard deviation.

3.2.2 | Varying SD and constant mean

The different PSDs having constant mean (47.5 ± 2.5 nm) and different SDs (viz., 7 and 21) using normal PDF are compared in Figure 8A. For PSD with SD = 7 takes into account the pore width from 33 to 68 nm and the PSD with SD = 21 considers the pore width from 14 to 90 nm.

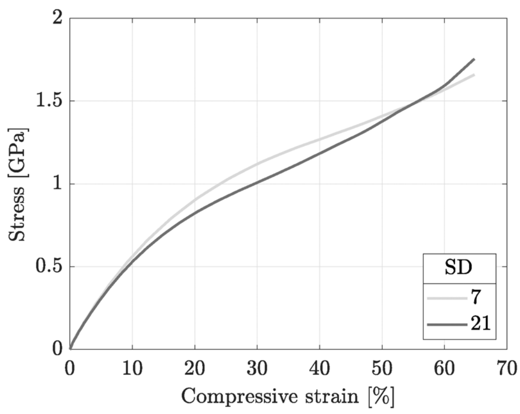

FIGURE 9 Comparison of the bulk response of the structure with PSDs corresponding to Figure 8A, for different SD and constant mean pore width. PSD, pore size distribution; SD, standard deviation.

In order to study only the influence of the PSD on the bulk response, the PDFs were chosen such that the structures have the same CWD (4.5 ± 0.05 nm) and RVE size (400 ± 10 nm) with the same porosity fraction. As the porosity of both the structure with SD = 7 & 21 is the same, we notice the same bulk elastic stiffness from Figure 9. However, there is a significant difference in the bulk response of the structures at large compressive strain. From comparing the cumulative PSD in Figure 8B, we see that the volume contribution of larger cells in PSD with larger SD is more compared to PSD with smaller SD. Due to the contribution of larger cells, the structure with larger SD shows softening response above the compressive strain of 10%. In addition, SD = 21 shows earlier densification resulting in a stiffer response which is due to denser smaller cells in the structure.

4 | CONCLUSION

In this work, the influence of different geometric parameters, namely, PSD, porosity and pore wall diameter, on the behavior of the computational model is investigated to understand the structure-property relation of open-porous cellular-like materials. An RVE of any size inheriting the complete PSD shows a similar bulk response. PSD and porosity are the most important parameter which highly influences the bulk response of the structure. A Computationally feasible minimum RVE size can be obtained based on the convergence study of effective geometric and bulk properties. In the modeling of porous material, porosity is sufficient to describe the linear elastic behavior of porous material using a power scaling law [1]. However, PSD plays a vital role in describing the complete description of stress-strain response, namely elastic, plateau, and densification regimes. CWD and the RVE size are dependent on PSD and solid fraction and are therefore, less significant. On the other hand, one needs to necessarily account for both the PSD and the solid fraction during the synthesis of the porous materials tailored for a specific application, as they are primary geometric properties that influence the bulk mechanical response.

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